JS 10/22/21
RJA 2/18/22

Fate Report for Case # P-19-0002

Fate
Summary Statement

Fate Summary Statement: P-19-0002
FATE:
[redacted] with MP = [redacted] °C (M)
log Kow = 4.35 (E)
S = 1.28 mg/L
at 25 °C (E)
VP < 1.0E-6 torr at 25 °C (E)
BP > 400 °C
(E)
H < 1.00E-8 (E)
log Koc = 7.08 (E)
log Fish BCF = 0.50 (3)
(E)
log Fish BAF = 2.40 (250) (E)
POTW removal (%) = 90 via
sorption and biodeg
Time for complete ultimate aerobic biodeg =
wk
Sorption to soils/sediments = strong
PBT Potential: P2B1
FATE:
Migration to ground water = negl
Bioconcentration factor to be put into
E-FAST: 3

PMN Material:
Overall wastewater treatment removal is
90% via sorption and biodegradation.
Sorption to sludge is moderate
to strong based on the estimated physical-chemical properties from EPISUITE. There was disagreement between the octanol-water partition coefficient and the soil adsorption coefficient.
Air Stripping
(Volatilization to air) is negligible based on the estimated
physical-chemical properties from EPISUITE.
Removal by
biodegradation in wastewater treatment is high based on the BIOWIN model estimates from EPISUITE.
The aerobic aquatic biodegradation half-life
is less than two months based on the BIOWIN model estimates from EPISUITE.

The anaerobic aquatic biodegradation half-life is two to six months based on the aerobic biodegradation half-life. The anaerobic biodegradation half-life is projected to be greater than or equal to the aerobic biodegradation half-life.

Sorption to soil and sediment is
strong based on the estimated physical-chemical properties from EPISUITE.

Migration to groundwater is negligible, mitigated by biodegradation.

PMN Material:
Persistent (P2) based on the anaerobic
biodegradation half-life.
Low Bioaccumulation (B1) based on the
BCFBAF model estimates from EPISUITE (BCF: 3 and BAF: 250).

Bioconcentration/Bioaccumulation factor to be put into E-Fast:
3.

CBI: [redacted]
Fate Assessor: Lynch, David
SMILES: [redacted]

Physical Properties

Property	Measured/Calculated Value	EPI
Molecular Form:	[redacted]	[redacted]
Molecular Wt.:		[redacted] g/mol
% < 500:		
% < 1000:		

Property	Measured Value	Method	Estimated Value	Method	EPI
Melting Point:	[redacted]				NaN °C (Exp.) 349.8399963378906 °C (Est., Joback) 349.8399963378906 °C (Est., Gold) 349.8399963378906 °C (Est., Selected)
Boiling Point:			>400		NaN °C (Exp.) 806.88 °C (Est.) 1080.037353515625 °K (Est.)
BP Pressure:					
Vapor Pressure:			<0.000001		NaN mmHg (Exp.) 6.465034737683413E-31 Pa

Property	Measured Value	Method	Estimated Value	Method	EPI
					(Est., Antoine) 4.8491882342624714E-33 mmHg (Est., Antoine) 5.5084141387951636E-18 Pa (Est., Grain) 4.131661795348977E-20 mmHg (Est., Grain) 3.321187389468266E-17 Pa (Est., Mackay) 2.4911022857954917E-19 mmHg (Est., Mackay) 5.5084141387951636E-18 Pa (Est., Selected) 4.131661795348977E-20 mmHg (Est., Selected) 2.8229349605452853E-14 Pa (Est., SubCooled) 2.117381197810778E-16 mmHg (Est., SubCooled)
Water Solubility:			0.00128		NaN (Exp.) 0.11237538605928421 (Est.)
Log P:			4.35		
Log Kow:					NaN (Exp.) 4.35 (Est.)
Log Koc:	NaN				16.299419043084967 (Est., log (MCI)) 6.151284854161446 (Est., log (Kow)) 1.1988028E7 L/kg (Est., MCI) 469.32000732421875 L/kg (Est., Kow)
Log BCF:					3.16 L/kg wet-wt
Henry's Law:					NaN atm-m3/mole (Exp.) 3.2458455398784197E-26 atm-m3/mole (Est., Bond) 3.224462401929075E-27 atm-

Property	Measured Value	Method	Estimated Value	Method	EPI
					m3/mole (Est., Group)

pH:	
pH Comment:	

Fate Analysis

Hydrolysis (t1/2, da):		**Volatilization (t1/2) - River (hr):**		**Volatilization (t1/2) - Lake (da):**	
Atm Ox Potential (t1/2)OH (hr):	1.058558863305411	**Atm Ox Potential (t1/2)O3 (hr):**	0.0	**Atm Ox Potential (t1/2) Total (hr):**	
MITI Linear:	1.2000000476837158	**MITI NonLinear:**	0.8999999761581421		
Biodeg Linear:	1.5	**Biodeg NonLinear:**	1.0		
Biodeg Survey ult:	2.299999952316284	**Biodeg Survey Prim:**	3.299999952316284		
STP (% removal) Total:	47.754792748533504%	**STP (% removal) Biodeg:**	0.45881470795894014%		
STP (% removal) Ads:	47.29597305029583%	**STP (% removal) Air:**	2.856846531813672E-21%		

Rationales

Removal in Wastewater Treatment:	
Atmospheric Oxidation:	
Hydrolysis:	
Photolysis:	
Aerobic Biodegradation:	
Anaerobic Biodegradation:	
Sorption to Soil and Sediment:	
Migration to Groundwater:	
Persistence - Air:	

Persistence - Water:	
Volatilization from Water:	
Soil:	
Sediment:	
Other:	
Standard:	
Bioaccumulation:	

PBT Ratings

Persistence	Bioaccumulation	Toxicity	PBT Comments
2	1		

Exposure-Based Testing

Exposure-Based Testing:	

Fate Ratings
Removal in WWT/POTW (Overall):

Removal in WWT/POTW (Overall):	90

Condition	Rating Values	Rating Description				Comment
		1	2	3	4	
WWT/POTW Sorption:	2-3	Low	Moderate	Strong	V. Strong	
WWT/POTW Stripping:	4	Extensive	Moderate	Low	Negligible	
Biodegradation Removal:	2	Unknown	High	Moderate	Negligible	
Biodegradation Destruction:		Unknown	Complete	Partial	—	
Aerobic Biodeg Ult:	2	<= Days	Weeks	Months	> Months	
Aerobic Biodeg Prim:		<= Days	Weeks	Months	> Months	
Anaerobic Biodeg Ult:	3	<= Days	Weeks	Months	> Months	
Anaerobic Biodeg Prim:		<= Days	Weeks	Months	> Months	
		<= Minutes	Hours	Days	>= Months	

Condition	Rating Values	Rating Description				Comment
		1	2	3	4	
Hydrolysis (t1/2 at pH 7,25C) A:						
Hydrolysis (t1/2 at pH 7,25C) B:		<= Minutes	Hours	Days	>= Months	
Sorption to Soils/Sediments:	2	V. Strong	Strong	Moderate	Low	
Migration to Ground Water:	1	Negligible	Slow	Moderate	Rapid	
Photolysis A, Direct:		Negligible	Slow	Moderate	Rapid	
Photolysis B, Indirect:		Negligible	Slow	Moderate	Rapid	
Atmospheric Ox A, OH:		Negligible	Slow	Moderate	Rapid	
Atmospheric Ox B, O3:		Negligible	Slow	Moderate	Rapid	

Bio Comments:

Bio Comments:	Fish log BAF = 2.40 (250). The fugacity spreadsheet and the EPI output file for the PMN material are attached.

Fate Comments:

Fate Comments:	

Comments/Telephone Log

Artifact	Update/Upload Time
[redacted]	[redacted]